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cis-($\eta^5\text{-C}_5\text{Me}_5$)Re(NO)(PPh₃)(C≡CC(OMe)=)W(PMe₃)(CO)₄ (8). A 5 mm NMR tube was charged with **3** (0.020 g, 0.020 mmol), THF (0.5 mL), and PMe₃ (0.0052 mL, 0.050 mmol), placed in a Pyrex ice bath, and irradiated (external Hanovia 450 W lamp, 0 °C, 2.5 h; >95% conversion by ³¹P NMR). Hexane (5 mL) was added. Chromatography (N₂, Florisil washed with aq. NH₄OH; hexane → 5:1 v/v hexane/THF) gave a bright red band. Solvent was removed by oil pump vacuum to give **8** as deep red microcrystals (0.014 g, 0.013 mmol, 65%). IR (cm⁻¹, CH₂Cl₂/KBr) ν_{CO} 2003/2001 m, 1933/1930 m, ν_{CO} + ν_{C≡C} 1873/1866 vs-br, ν_{NO} 1657/1657 m.

NMR (C₆D₆):⁵⁰ ¹H 7.57-7.45 (m, 6H of 3C₆H₅), 7.15-6.90 (m, 9H of 3C₆H₅), 3.25 (s, OCH₃), 1.67 (s, C₅(CH₃)₅), 1.29 (d, J_{HP} = 7.4, P(CH₃)₃); ¹³C{¹H} 264.6 (d, J_{CPMe} = 11.4, C=W), 212.1 (d, J_{CPMe} = 6.1, CO cis to PMe₃), 211.4 (d, J_{CPMe} = 24.0, CO trans to PMe₃), 205.4 (d, J_{CPMe} = 7.2, CO cis to PMe₃), 204.9 (d, J_{CPMe} = 7.7, CO cis to PMe₃), 191.0 (d, J_{CPPh} = 13.1, ReCC), 154.8 (s, ReCC), 134.0 (d, J_{CPPh} = 10.4, *o*-Ph), 130.6 (s, *p*-Ph), 128.7 (d, J_{CPPh} = 10.4, *m*-Ph), 103.1 (s, C₅(CH₃)₅), 61.3 (s, OCH₃), 20.4 (d, J_{CPMe} = 24.9, P(CH₃)₃), 10.1 (s, C₅(CH₃)₅); ³¹P{¹H} 22.5 (s, PPh₃), -32.3 (s, PMe₃).

($\eta^5\text{-C}_5\text{Me}_5$)Re(NO)(PPh₃)(C≡CC≡CC(OMe)=)Mn(CO)₂($\eta^5\text{-C}_5\text{Br}_5$) (19). Complex **13** (0.066 g, 0.10 mmol), THF (5 mL), *n*-BuLi (0.055 mL, 2.3 M in hexane), Mn(CO)₃($\eta^5\text{-C}_5\text{Br}_5$) (0.060 g, 0.10 mmol;¹⁷ in 3 mL THF), and Me₃O⁺BF₄⁻ (0.044 g, 0.30 mmol) were combined in a procedure analogous to that for **16**. An identical workup gave **19** as a dark blue sticky residue, which solidified over the course of 4-5 h under oil pump vacuum (0.061 g, 0.055 mmol, 55%; contaminated with a small amount of Mn(CO)₃($\eta^5\text{-C}_5\text{Br}_5$) by IR), mp 122-125 °C. IR (cm⁻¹, CH₂Cl₂/KBr) ν_{C≡C} 2057/2054 m, ν_{CO} 1965/1963 vs, 1924/1925 m, ν_{NO} 1657/1654 s. UV-vis (2.6 × 10⁻⁵ M)⁴⁸ 264 sh (20100), 320 (11600), 384 (8500), 566 (11400), 588 sh (11000).

NMR (CD₂Cl₂):⁵⁰ ¹H 7.80-7.10 (m br, 3C₆H₅), 4.08 (s, OCH₃), 1.79 (s, C₅(CH₃)₅); ¹³C-{¹H} 288.9 (s, C=Mn), 228.9 (s, CO), 228.8 (s, CO), 169.7 (d, J_{CP} = 11.4, ReCC), 134.1 (d, J_{CP} = 10.2, *o*-Ph), 131.0 (s, *p*-Ph), 128.8 (d, J_{CP} = 10.1, *m*-Ph), 127.6, 116.7, 82.6 (3 s, ReCCCC), 102.7 (s, C₅(CH₃)₅), 89.8 (s, C₅Br₅), 63.9 (s, OCH₃), 10.2 (s, C₅(CH₃)₅); ³¹P{¹H} 21.2 (s).

Table SMI. Summary of Crystallographic Data for $(\eta^5\text{-C}_5\text{Me}_5)\text{Re}(\text{NO})(\text{PPh}_3)(\text{C}\equiv\text{CC}(\text{OMe})=\text{W})(\text{CO})_5$ (**3**) and $[(\eta^5\text{-C}_5\text{Me}_5)\text{Re}(\text{NO})(\text{PPh}_3)(\text{CCC})\text{Mn}(\text{CO})_2(\eta^5\text{-C}_5\text{H}_5)]^+ \text{BF}_4^- \cdot (\text{CH}_2\text{Cl}_2)_{0.5}$ (**9**• $(\text{CH}_2\text{Cl}_2)_{0.5}$)

	3	9 • $(\text{CH}_2\text{Cl}_2)_{0.5}$
Formula	$\text{C}_{37}\text{H}_{33}\text{NO}_7\text{PReW}$	$\text{C}_{77}\text{H}_{72}\text{B}_2\text{Cl}_2\text{F}_8\text{N}_2\text{Mn}_2\text{O}_6\text{P}_2\text{Re}_2^{\text{a}}$
Formula weight	1004.702	1910.18
Crystal system	triclinic	triclinic
Space group	$\bar{\text{P}}\bar{1}$	$\bar{\text{P}}\bar{1}$
Cell dimensions		
\underline{a} , Å	13.125(2)	8.732(1)
\underline{b} , Å	13.837(3)	15.248(4)
\underline{c} , Å	10.880(2)	28.850(5)
α , deg	109.16(2)	84.68(2)
β , deg	92.48(2)	97.01(1)
γ , deg	77.80(2)	102.40(2)
V, Å ³	1823.55	3714.80
Z	2	2
temp of collection (°C)	16	-125
d _{calc} , g/cm ³	1.830	1.71
d _{found} , g/cm ³ (22 °C)	1.805	1.701
Crystal dimensions, mm	0.42 x 0.32 x 0.15	0.31 x 0.22 x 0.06
Radiation (Å)	Mo K _α (0.70930)	Mo K _α (0.70930)
Data collection method	θ - 2θ	θ - 2θ
Scan speed, deg/min	variable	variable
Reflections measured	6765	12998
Range/indices (h, k, l)	0 15, -15 15, -12 12	0 9, -18 18, -33 33
2θ limit, deg	2.0 - 50.0	34.0 - 48.0
Scan width	0.80 + 0.34 Tan θ	0.80 + 0.34 Tan θ
Standard reflections check	1 X-ray hour	1 X-ray hour
Total unique data	6394	12051
Observed data, I > 3σ(I)	5207	8935
Abs. coefficient, cm ⁻¹	66.71	37.98
Min transmission, %	49.88	62.54
Max. transmission, %	99.79	99.99
No. of variables	433	928
Goodness of fit	0.90	2.04
$R = \sum F_O - F_C / \sum F_O $	0.029	0.054
$R_w = \sum F_O - F_C w^{1/2} / \sum F_O w^{1/2}$	0.033	0.072
Δ/σ (max)	0.002	0.011
Δρ (max), e/Å ³	1.909	2.131

^aFor two independent molecules in the unit cell

Table SM2. Atomic Coordinates for non-Hydrogen Atoms of
 $[(\eta^5\text{-C}_5\text{Me}_5)\text{Re}(\text{NO})(\text{PPh}_3)(\text{CCC})\text{Mn}(\text{CO})_2(\eta^5\text{-C}_5\text{H}_5)]^+ \text{BF}_4^- \cdot (\text{CH}_2\text{Cl}_2)_{0.5}$
 $(9 \cdot (\text{CH}_2\text{Cl}_2)_{0.5})$.

Atom	x(sd)	y(sd)	z(sd)
Re	0.90497(5)	0.72457(3)	0.10020(1)
Re'	0.46913(4)	0.32705(2)	0.32831(1)
Mn	0.9981(2)	1.1041(1)	0.17571(7)
Mn'	0.4392(2)	-0.0825(1)	0.32431(7)
P'	0.3798(3)	0.2787(2)	0.4038(1)
P	1.0954(3)	0.6654(2)	0.1549(1)
O1'	0.1663(9)	0.3661(5)	0.2840(3)
O1	0.6496(9)	0.6240(5)	0.1540(3)
O2'	0.747(1)	-0.0627(6)	0.2863(3)
O2	0.960(1)	1.1837(7)	0.0795(4)
O3	0.658(1)	1.0726(7)	0.1875(4)
O3'	0.263(1)	-0.1025(6)	0.2302(4)
N	0.7564(9)	0.6658(6)	0.1344(4)
N'	0.2821(9)	0.3422(5)	0.3040(3)
C1'	0.603(1)	0.4273(8)	0.2761(5)
C1	0.749(2)	0.702(1)	0.0328(5)
C2'	0.696(1)	0.3610(8)	0.2911(4)
C2	0.822(2)	0.7935(9)	0.0318(6)
C3'	0.742(1)	0.3654(7)	0.3405(4)
C3	0.984(2)	0.7994(9)	0.0309(5)
C4'	0.680(1)	0.4367(7)	0.3560(4)
C4	1.011(1)	0.7105(9)	0.0312(4)
C5	0.864(2)	0.6501(8)	0.0335(5)
C5'	0.600(1)	0.4750(7)	0.3151(4)
C6'	0.540(2)	0.448(1)	0.2260(4)
C6	0.570(2)	0.661(2)	0.0319(7)
C7'	0.747(1)	0.2997(9)	0.2603(5)
C7	0.735(2)	0.871(1)	0.0286(8)
C8	1.109(3)	0.887(1)	0.0236(6)
C8'	0.853(1)	0.3138(7)	0.3682(4)
C9'	0.720(1)	0.4736(8)	0.4040(4)
C9	1.173(2)	0.690(1)	0.0248(6)
C10'	0.530(1)	0.5576(7)	0.3146(5)
C10	0.836(3)	0.550(1)	0.0269(6)
C11'	0.294(1)	0.3598(7)	0.4285(4)
C11	1.128(1)	0.5588(7)	0.1383(4)
C12	1.278(1)	0.5522(7)	0.1284(4)
C12'	0.226(1)	0.3386(8)	0.4711(4)
C13	1.298(1)	0.4709(8)	0.1132(5)
C13'	0.158(1)	0.4041(8)	0.4887(5)
C14'	0.154(1)	0.4850(8)	0.4639(4)
C14	1.170(2)	0.4009(7)	0.1081(4)
C15'	0.219(1)	0.5059(7)	0.4205(4)
C15	1.020(1)	0.4071(8)	0.1171(5)
C16	1.000(1)	0.4886(7)	0.1326(4)
C16'	0.289(1)	0.4424(7)	0.4032(5)
C21	1.292(1)	0.7329(7)	0.1674(4)
C21'	0.533(1)	0.2491(7)	0.4474(4)

C22	1.389(1)	0.7125(7)	0.2072(5)
C22'	0.589(1)	0.2958(7)	0.4876(4)
C23'	0.713(1)	0.2697(8)	0.5180(4)
C23	1.540(1)	0.7634(7)	0.2165(5)
C24	1.597(1)	0.8354(8)	0.1860(4)
C24'	0.782(1)	0.2025(8)	0.5074(5)
C25	1.498(2)	0.8588(9)	0.1455(5)
C25'	0.729(1)	0.1556(8)	0.4671(5)
C26'	0.601(1)	0.1783(7)	0.4366(5)
C26	1.345(1)	0.8082(8)	0.1360(5)
C31'	0.226(1)	0.1756(7)	0.4055(4)
C31	1.031(1)	0.6415(7)	0.2130(4)
C32'	0.116(1)	0.1579(8)	0.3666(5)
C32	1.053(1)	0.5635(8)	0.2400(4)
C33	1.013(1)	0.5506(8)	0.2870(4)
C33'	-0.001(1)	0.0797(8)	0.3675(5)
C34	0.954(1)	0.6137(9)	0.3052(4)
C34'	-0.007(1)	0.0203(8)	0.4067(5)
C35'	0.101(1)	0.0373(9)	0.4435(6)
C35	0.933(1)	0.6939(8)	0.2787(4)
C36'	0.220(1)	0.1154(8)	0.4453(5)
C36	0.972(1)	0.7064(7)	0.2316(4)
C40	0.950(1)	0.8365(7)	0.1286(4)
C40'	0.456(1)	0.2012(7)	0.3212(4)
C41'	0.457(1)	0.1195(7)	0.3160(4)
C41	0.972(1)	0.9159(7)	0.1428(4)
C42'	0.452(1)	0.0347(7)	0.3176(4)
C42	0.983(1)	0.9968(7)	0.1568(4)
C50	1.123(2)	1.0872(9)	0.2444(5)
C50'	0.385(2)	-0.088(1)	0.3942(5)
C51'	0.510(2)	-0.135(1)	0.3924(5)
C51	1.230(2)	1.1106(9)	0.2104(5)
C52'	0.451(2)	-0.2079(9)	0.3648(6)
C52	1.216(2)	1.196(1)	0.1882(5)
C53	1.102(2)	1.2270(8)	0.2096(5)
C53'	0.293(2)	-0.208(1)	0.3491(7)
C54	1.042(2)	1.1603(8)	0.2423(5)
C54'	0.256(2)	-0.132(1)	0.3681(6)
C60	0.972(2)	1.1538(8)	0.1163(5)
C60'	0.627(1)	-0.0731(7)	0.3018(5)
C61'	0.333(1)	-0.0953(7)	0.2663(5)
C61	0.790(2)	1.0853(8)	0.1826(5)
Cl1	0.3199(6)	0.0574(4)	0.1027(2)
Cl2	0.5766(6)	0.0520(4)	0.0505(2)
F1	0.9672(8)	0.7038(5)	0.4086(3)
F2	0.8539(8)	0.8043(5)	0.4385(3)
F3	0.7035(9)	0.6856(5)	0.4060(4)
F4	0.839(1)	0.7972(6)	0.3614(3)
F1'	0.364(1)	0.5821(7)	0.8838(6)
F2'	0.336(1)	0.691(1)	0.9279(3)
F3'	0.351(2)	0.7163(9)	0.8537(4)
F4'	0.565(1)	0.7062(8)	0.9025(5)
C70	0.495(2)	0.119(1)	0.0805(7)
B	0.838(2)	0.7463(9)	0.4031(6)
B'	0.404(2)	0.671(1)	0.8936(7)

Table SM3. Anisotropic Displacement Parameters for **9•(CH₂Cl₂)_{0.5}**

Atom	<i>U</i> ₁₁ (sd)	<i>U</i> ₂₂ (sd)	<i>U</i> ₃₃ (sd)	<i>U</i> ₁₂ (sd)	<i>U</i> ₁₃ (sd)	<i>U</i> ₂₃ (sd)
Re	0.0251(2)	0.0204(2)	0.0247(2)	0.0067(2)	0.0044(2)	-0.0011(2)
Re'	0.0146(2)	0.0175(2)	0.0195(2)	0.0016(1)	0.0010(2)	-0.0027(2)
Mn	0.044(1)	0.0276(8)	0.035(1)	0.0082(7)	-0.0010(8)	-0.0065(7)
Mn'	0.0301(9)	0.0218(7)	0.046(1)	0.0052(6)	0.0009(8)	-0.0048(8)
P'	0.018(1)	0.019(1)	0.023(1)	0.002(1)	0.003(1)	-0.002(1)
P	0.024(1)	0.021(1)	0.023(1)	0.003(1)	0.006(1)	0.000(1)
O1'	0.030(4)	0.042(4)	0.042(5)	0.018(3)	-0.013(4)	-0.009(4)
O1	0.029(4)	0.039(4)	0.058(5)	-0.001(3)	0.018(4)	0.001(4)
O2'	0.038(5)	0.066(5)	0.039(5)	0.001(4)	-0.001(4)	-0.017(4)
O2	0.099(8)	0.052(6)	0.049(6)	0.011(5)	0.002(6)	-0.001(5)
O3	0.056(6)	0.070(6)	0.081(7)	0.017(5)	0.006(5)	-0.018(5)
O3'	0.059(5)	0.057(5)	0.063(6)	0.026(4)	-0.019(5)	-0.029(4)
N	0.015(4)	0.026(4)	0.046(6)	0.004(3)	0.001(4)	0.005(4)
N'	0.023(4)	0.012(3)	0.022(4)	0.001(3)	0.014(3)	0.009(3)
C1'	0.021(5)	0.036(6)	0.053(7)	-0.003(5)	0.014(5)	-0.002(6)
C1	0.036(7)	0.10(1)	0.037(8)	0.018(7)	0.001(6)	-0.004(8)
C2'	0.019(5)	0.040(6)	0.025(5)	-0.004(4)	0.005(4)	-0.009(5)
C2	0.061(8)	0.064(7)	0.07(1)	0.035(6)	0.007(7)	0.032(7)
C3'	0.017(5)	0.024(5)	0.047(7)	-0.002(4)	0.005(5)	0.002(5)
C3	0.08(1)	0.033(7)	0.043(8)	-0.012(7)	0.006(7)	-0.006(6)
C4'	0.018(5)	0.033(5)	0.027(5)	0.000(4)	0.006(4)	-0.010(4)
C4	0.031(6)	0.065(7)	0.037(7)	0.022(5)	0.010(5)	-0.011(6)
C5	0.049(7)	0.034(6)	0.048(8)	0.003(5)	0.009(6)	0.007(6)
C5'	0.021(5)	0.021(5)	0.040(6)	-0.006(4)	0.004(5)	0.008(5)
C6'	0.052(8)	0.081(9)	0.017(6)	-0.012(7)	-0.003(6)	0.023(6)
C6	0.031(8)	0.22(2)	0.06(1)	0.00(1)	-0.008(8)	-0.00(1)
C7'	0.045(7)	0.055(7)	0.051(7)	0.005(6)	0.020(6)	-0.018(6)
C7	0.22(1)	0.14(1)	0.09(2)	0.145(8)	0.02(1)	0.03(1)
C8	0.16(2)	0.09(1)	0.036(9)	-0.07(1)	0.01(1)	0.004(9)
C8'	0.027(5)	0.030(5)	0.033(6)	0.006(4)	-0.007(5)	0.007(5)
C9'	0.036(6)	0.039(6)	0.026(6)	-0.010(5)	0.003(5)	-0.010(5)
C9	0.051(7)	0.16(1)	0.07(1)	0.065(7)	0.011(7)	-0.019(9)
C10'	0.022(5)	0.021(5)	0.077(9)	0.005(4)	0.000(6)	0.011(6)
C10	0.18(2)	0.039(8)	0.049(9)	-0.00(1)	0.02(1)	-0.016(7)
C11'	0.017(5)	0.027(5)	0.027(5)	0.002(4)	0.002(4)	-0.006(4)
C11	0.032(6)	0.026(5)	0.032(6)	0.008(4)	0.002(5)	0.002(5)
C12	0.042(6)	0.026(5)	0.044(7)	0.013(4)	0.005(5)	-0.009(5)
C12'	0.029(5)	0.043(6)	0.029(6)	0.003(5)	0.012(4)	-0.010(5)
C13	0.051(7)	0.037(6)	0.044(7)	0.016(5)	0.010(6)	-0.003(5)
C13'	0.026(6)	0.036(6)	0.055(8)	0.009(4)	0.005(5)	-0.012(5)
C14'	0.034(6)	0.035(6)	0.040(6)	0.007(4)	0.013(5)	-0.011(5)
C14	0.071(8)	0.026(5)	0.026(6)	0.015(5)	-0.004(6)	-0.005(5)
C15'	0.035(6)	0.032(5)	0.045(7)	0.010(4)	0.015(5)	-0.008(5)
C15	0.059(7)	0.038(6)	0.033(7)	0.024(5)	-0.014(6)	-0.008(5)
C16	0.030(6)	0.029(5)	0.038(7)	0.000(5)	-0.008(5)	-0.010(5)
C16'	0.022(5)	0.025(5)	0.052(7)	0.003(4)	0.000(5)	-0.008(5)
C21	0.027(5)	0.024(5)	0.039(6)	-0.004(4)	0.016(4)	-0.011(4)
C21'	0.016(5)	0.021(5)	0.029(6)	-0.004(4)	0.003(4)	-0.003(4)

C22	0.018(5)	0.033(5)	0.061(8)	0.011(4)	-0.009(5)	-0.013(5)
C22'	0.032(6)	0.028(5)	0.029(6)	-0.007(5)	-0.004(5)	-0.003(5)
C23'	0.037(6)	0.039(6)	0.034(7)	0.001(5)	-0.002(5)	-0.004(5)
C23	0.020(5)	0.027(5)	0.070(8)	0.001(4)	0.011(5)	-0.011(6)
C24	0.037(6)	0.051(7)	0.039(7)	0.003(5)	0.004(5)	-0.024(5)
C24'	0.033(6)	0.039(6)	0.039(7)	0.007(5)	-0.008(5)	-0.009(5)
C25	0.042(7)	0.045(7)	0.071(9)	-0.022(6)	0.021(6)	-0.011(7)
C25'	0.035(6)	0.040(6)	0.041(7)	0.007(5)	-0.002(6)	0.001(6)
C26'	0.031(5)	0.033(5)	0.056(8)	0.018(4)	0.010(5)	0.012(5)
C26	0.035(6)	0.043(6)	0.043(7)	-0.007(5)	0.012(5)	-0.013(5)
C31'	0.020(5)	0.015(4)	0.052(7)	-0.002(4)	0.011(5)	-0.004(5)
C31	0.017(5)	0.028(5)	0.027(6)	-0.006(4)	0.000(4)	-0.003(5)
C32'	0.023(6)	0.030(6)	0.061(8)	-0.005(5)	0.011(5)	-0.005(6)
C32	0.027(5)	0.040(6)	0.022(6)	0.006(5)	0.008(4)	0.008(5)
C33	0.031(6)	0.046(6)	0.024(6)	0.004(5)	0.005(5)	0.002(5)
C33'	0.035(6)	0.037(6)	0.068(8)	-0.021(5)	0.021(6)	-0.016(6)
C34	0.018(5)	0.053(7)	0.035(7)	-0.011(5)	-0.002(5)	-0.008(6)
C34'	0.035(6)	0.030(6)	0.095(9)	-0.006(5)	0.041(5)	-0.011(6)
C35'	0.038(6)	0.039(7)	0.10(1)	0.008(5)	0.032(6)	0.010(7)
C35	0.022(5)	0.047(6)	0.026(6)	-0.004(5)	0.002(5)	-0.015(5)
C36'	0.032(6)	0.037(6)	0.055(8)	0.002(5)	0.015(5)	0.011(6)
C36	0.024(5)	0.035(6)	0.025(6)	-0.004(5)	0.003(5)	-0.004(5)
C40	0.026(5)	0.026(5)	0.041(6)	0.007(4)	0.014(5)	0.002(5)
C40'	0.018(5)	0.030(5)	0.020(5)	0.006(4)	-0.004(4)	-0.012(4)
C41'	0.027(6)	0.039(6)	0.019(5)	0.003(5)	-0.006(5)	-0.011(5)
C41	0.037(6)	0.024(5)	0.047(7)	0.004(5)	0.004(5)	-0.008(5)
C42'	0.030(5)	0.025(5)	0.025(6)	0.009(4)	-0.003(5)	-0.006(4)
C42	0.037(6)	0.033(5)	0.030(6)	0.011(4)	0.004(5)	-0.001(5)
C50	0.048(7)	0.060(7)	0.035(7)	0.016(6)	-0.012(6)	-0.010(6)
C50'	0.11(1)	0.056(8)	0.069(8)	0.032(7)	0.063(6)	0.038(7)
C51'	0.047(8)	0.050(8)	0.062(9)	-0.003(6)	0.012(7)	0.009(7)
C51	0.042(7)	0.054(8)	0.038(7)	-0.004(6)	-0.007(6)	-0.000(6)
C52'	0.053(8)	0.040(7)	0.07(1)	0.013(6)	0.003(7)	0.016(7)
C52	0.057(9)	0.054(8)	0.052(9)	-0.011(7)	-0.018(7)	-0.008(7)
C53	0.068(9)	0.031(6)	0.054(8)	0.007(6)	-0.011(7)	-0.019(6)
C53'	0.038(8)	0.043(8)	0.12(1)	-0.004(6)	-0.017(9)	0.011(9)
C54	0.082(9)	0.040(6)	0.044(8)	0.026(6)	-0.014(7)	-0.013(6)
C54'	0.051(8)	0.096(9)	0.11(1)	0.023(7)	0.035(7)	0.085(7)
C60	0.078(9)	0.034(6)	0.029(7)	0.004(6)	0.002(6)	-0.003(5)
C60'	0.042(6)	0.026(5)	0.048(7)	0.008(5)	-0.008(6)	-0.019(5)
C61'	0.047(7)	0.026(5)	0.057(8)	0.014(5)	0.002(6)	-0.013(5)
C61	0.054(7)	0.039(6)	0.049(8)	0.009(5)	0.003(6)	-0.014(6)
Cl1	0.079(3)	0.117(4)	0.095(3)	0.008(3)	0.022(2)	-0.027(3)
Cl2	0.108(3)	0.116(4)	0.154(5)	0.049(2)	0.065(3)	0.024(3)
F1	0.042(4)	0.066(4)	0.051(5)	0.024(3)	-0.003(3)	-0.006(4)
F2	0.053(4)	0.043(4)	0.044(4)	0.008(3)	0.006(3)	-0.001(3)
F3	0.039(4)	0.047(4)	0.162(9)	0.005(4)	-0.035(5)	-0.021(5)
F4	0.129(6)	0.089(5)	0.028(4)	0.063(4)	0.008(4)	0.010(4)
F1'	0.074(6)	0.079(7)	0.27(1)	0.019(5)	0.070(7)	0.003(9)
F2'	0.058(6)	0.26(1)	0.040(5)	0.008(7)	0.007(4)	-0.037(7)
F3'	0.30(2)	0.12(1)	0.047(7)	0.02(1)	-0.039(9)	0.005(7)
F4'	0.067(5)	0.098(7)	0.23(1)	0.022(5)	0.067(6)	0.001(8)
C70	0.07(1)	0.11(1)	0.10(1)	0.01(1)	0.035(9)	0.00(1)

B'	0.035(7)	0.09(1)	0.10(1)	0.016(7)	0.037(7)	-0.02(1)
B	0.043(8)	0.028(6)	0.045(9)	0.007(6)	-0.007(7)	-0.004(6)